

Methyl formate

107-31-3 | DTXSID5025609

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 1.78

Global applicability domain: Inside

Local applicability domain index: 9.57e-01

Confidence level: 6.06e-01

Nearest Neighbors from the Training Set

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Methyl formate

Measured: 1.75

Predicted: 1.78

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Propane

Measured: 0.97

Predicted: 1.60

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Acetonitrile

Measured: 2.31

Predicted: 1.96

Image not found

Nitromethane

Measured: 2.53

Predicted: 1.63

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Dimethyl ether

Measured: 1.37

Predicted: 1.58